

2588-Pos Board B607**Applications of Artificial Neural Networks to Proton and Electron Impact Ionization of Biologically Relevant Atoms and Molecules**Allison Harris¹, Jerry Darsey².¹Henderson State University, Arkadelphia, AR, USA, ²University of Arkansas at Little Rock, Little Rock, AR, USA.

We use Artificial Neural Networks (ANNs) to study proton and electron impact single ionization of biologically relevant atoms and molecules. In these processes, an incident proton or electron collides with a target atom or molecule causing a single electron to be ionized from the target. The process of ionization is biologically relevant for two reasons. Firstly, ionization results in reactive ions that are able to take part in damaging chemical reactions. Secondly, free electrons have been shown to result in DNA strand breaks, which can lead to cell death. While atomic and molecular collisions have been studied experimentally for decades, most of the available data is for noble gas atoms and small diatomic molecules. ANNs are computer programs that are trained to learn patterns in data and make predictions for cases where no data exists. They have been widely used in other fields, but this is one of the first applications of ANNs to atomic and molecular collision processes. In this work, we use the available experimental data to train the ANN, and then make predictions for biologically important target atoms and molecules where no data currently exists.

2589-Pos Board B608**Predicting Non-Specifically Bound Ions: Application to Bion Webserver and Beryllium Disease**

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Ions are important component of all living organisms. They affect the biological macromolecules either via direct binding or as a screening ion cloud. While some ion binding is highly specific and frequently associated with the function of the macromolecule, other ions bind to the protein surface non-specifically presumably because of electrostatic attraction being strong enough to immobilize them. Recently we developed a methodology utilizing DelPhi generated potential map to predict non-specifically bound ions and this methodology is now implemented into a webserver, the BION server. We use the BION to investigate the molecular mechanism associated with the beryllium disease via malfunctioning of HLA protein. The HLA-DP allele is known to cause chronic beryllium disease in humans while binding beryllium ion. Although several binding sites for beryllium ion to HLA-DP allele are already proposed, based on genetic susceptibility of organism and chemical properties of possible ion binding sites, they are still under intensive discussion. But as far as beryllium ion is expected to bind to the surface of protein, one may expect that this bonding is non-specific, and electrostatic force favors it. The HLA-DP with predicted bound ions is then investigated to reveal the effect of the ions on the protein flexibility to infer plausible mechanism of the disease. The work is supported by NIH, NIGMS, grant number 1R01GM093937.

2590-Pos Board B609**Charge Separation in Water on Strong Impacts and Recombination of Dispersed Ions**Frank Wiederschein¹, Esteban Vöhringer-Martinez², Bernd Abel³, Helmut Grubmüller¹.¹Max Planck Institute for Biophysical Chemistry, Göttingen, Germany,²Laboratorio de Química Teórica Computacional (QTC) Facultad de Química, Santiago de Chile, Chile, ³Leibniz Institute of Surface Modification, Leipzig, Germany.

Charge separation is a general phenomenon in nature. There has been vivid speculation and discussion about the mechanism of charge separation in condensed matter on strong impacts at small energies. Here we show that charge separation naturally occurs if water aggregates with embedded charge carriers, e.g. ions, encounter a high energy impact even though no plasma occurs and the involved kinetic energies are much below any molecular ionization energy. We find that the charge distribution in the fragments resulting from a strong impact can simply be described by a three step model.

The first level of the model is a simple statistical description of the resulting charge distribution at low salt concentrations by making usage of the Poisson distribution. The second step involves the mutual interaction between the charge particles in the condensed matter, which allows us to describe the charge process at higher salt concentrations. We achieved this by using implicit water Monte Carlo Simulation methods of the charged particles. Finally we included the full dynamics of the separation process into our model by using all-atom non-equilibrium Molecular Dynamics Simulations to describe the charge separation at high salt concentrations and high separation process velocities.

We present a microscopic model of the charging mechanism of fragments, that contributes to the understanding of a larger range of phenomena related to charges and charge separation in Nature.

To test our model we describe the ion yield of laser desorption experiments, i.e. LILBID, at different salt concentrations over six orders of magnitude. To accommodate for the specific setup of the experiment, we not only model the initial charge separation with our microscopic model but also account for ion recombination, which occurs between ion desorption and final ion detection.

2591-Pos Board B610**Effects of High Temperature on Desolvation Costs of Salt Bridges across Protein Binding Interfaces: Similarities and Differences between Implicit and Explicit Solvent Models**

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The role of salt bridges in protein-protein binding is largely determined by the costs of desolvating the oppositely charged members of the salt bridge upon binding. On the basis of Poisson-Boltzmann (PB) implicit solvent calculations, it has been proposed that the reduced desolvation penalties of salt bridges at high temperatures provide one explanation for the increased abundance of salt bridges in hyperthermophilic proteins. Here, for the first time, we directly compare the PB implicit solvent model with several explicit water models in computing the effects of extremely high temperature (i.e., 100 °C) on the desolvation penalties of salt bridges across protein-protein interfaces. With the exception of two outliers, the desolvation costs at 100 °C from implicit and explicit solvent calculations are of similar magnitudes and significantly reduced relative to 25 °C. The two outliers correspond to salt bridges that are both buried and part of a salt bridge network, a challenging case that should be considered in the development of fast solvation models.

2592-Pos Board B611**Developing and Applying Possim - a Fast Second-Order Polarizable Force Field for Biophysical Simulations**

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In this presentation we will report our progress in developing POSSIM (Polarizable Simulations with Second order Interaction Model) - a software suite and a complete fast polarizable force field for proteins and small molecules. It uses the second-order approximation formalism which permits to increase the computational speed in polarizable calculations by ca. an order of magnitude. We have significantly expanded the set of available parameters for protein residues and have now carried out simulations of realistic proteins and substituted polyalanine alpha-helices in gas-phase and aqueous solution.

2593-Pos Board B612**Optimization of a Coarse-Grained Force Field for Biological Simulations**Joseph Fogarty¹, See-Wing Chiu², Eric Jakobsson², Sagar Pandit¹.¹University of South Florida, Tampa, FL, USA, ²University of Illinois, Urbana, IN, USA.

The substantial gains in computational power over recent years have been the result of increased processor parallelization. For atomistic simulation, parallelization of spatial dimensions is a viable approach, leading to large length scale simulation. Parallelization of time, on the other hand, can be achieved by averaging of fast time scale motions. Coarse-Grained (CG) models accomplish this by replacing common groups of atoms with 0-dimension points (beads) and defining potentials between the beads. The challenge then is to choose functional forms and parameters for these potentials that accurately reproduce the behavior of equivalent atomistic and experimental systems. In this work, we consider the fundamental unit of water to be a bead representing four water molecules. The beads are made polarizable by the addition of a variable angular term between three charged points on each charge neutral site. Ionic beads are defined as equivalent to four water molecules solvating one atomistic ion. Further, building blocks of linear alkanes are beads of either 3 or 4 carbon units. Non-bonded, non-Coulomb interactions between beads are described by a modified Morse potential which addresses the complexity of multi-atomic beads by decoupling the short-range and long-range behavior. Instead of using a potential of relatively simple form, the comparatively complex potential is computed by lookup table. Optimization of force-field parameters is performed using FFOpt, an in-house software package. The method explores parameter space using Nelder-Mead, a simplex optimization algorithm. The error function for optimization is defined by comparison of CG simulation results to either those of atomistic simulation or experimental values. Analysis used is optimization includes density profile, diffusion coefficient, dielectric constant, and solvation free energies.